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AMPLIFICATION OF PRESSURE WAVES DURING VIBRATIONAL EQUILIBRATION OF EXCITED CHEMICAL REACTION PRODUCTS

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ABSTRACT

The Non-Equilibrium Zeldovich - von Neumann - Doring (NEZND) theory of self-sustaining detonation identified amplification of pressure wavelets during equilibration of vibrationally excited reaction products in the reaction zone as the physical mechanism by which exothermic chemical energy release sustains detonation waves. This mechanism leads to the formation of the well-known, complex three-dimensional structure of a self-sustaining detonation wave. This amplification mechanism is postulated to be a general property of subsonic and supersonic reactive flows occurring during: shock to detonation transition (SDT); hot spot ignition and growth; deflagration to detonation transition (DDT); flame acceleration by shock or compression waves; and acoustic (sound) wave amplification. The existing experimental and theoretical evidence for pressure wave amplification by chemical energy release into highly vibrationally excited product molecules under these reactive flow conditions is reviewed in this paper.

INTRODUCTION

The Non-Equilibrium Zeldovich - von Neumann – Doring (NEZND) theory was developed to identify the non-equilibrium chemical processes that precede and follow exothermic chemical energy

release within the reaction zones of self-sustaining detonation waves in gaseous, liquid and solid explosives¹⁻¹¹. Prior to the development of the NEZND model, the chemical energy released was merely treated as a heat of reaction in the conservation of energy equation in the Chapman-Jouguet (C-J)^{12,13}, Zeldovich–von Neumann-Döring (ZND)¹⁴⁻¹⁶, and curved detonation wave front theories¹⁷. NEZND theory has explained many experimentally determined detonation wave properties. These include: the induction time delays for the onset of chemical reaction; the rapid rates of the chain reactions that form the reaction product molecules; the de-excitation rates of the initially highly vibrationally excited products; the feedback mechanism that allows the chemical energy to sustain the leading shock wave front at an overall constant detonation velocity; and the establishment of the complex three-dimensional Mach stem structure of the leading shock wave fronts common to all detonation waves. Figure 1 illustrates the various processes that occur in the NEZND model of detonation in condensed phase explosives containing carbon, hydrogen, oxygen, and nitrogen atoms ($C_wH_xO_yN_z$). This feedback mechanism was identified as the amplification of pressure wavelets by “excess” vibrational energy initially present in highly vibrationally excited reaction product molecules (mainly CO_2 , CO , N_2 , and H_2O) as the wavelets propagate through the reaction zone and overtake the leading shock front⁷. This mechanism is discussed in detail in the next section. It appears to be a general physical phenomenon occurring in many types of reactive flows in which exothermic chemical reactions occur in the presence of acoustic, weak compression, and shock waves. The current experimental and theoretical understanding of wave amplification by non-equilibrium vibrationally excited molecules in various subsonic and supersonic reactive flows is discussed in the following sections.

THE MECHANISM OF PRESSURE WAVE AMPLIFICATION BY CHEMICAL ENERGY RELEASE

The physical mechanism by which “excess” vibrational energy communicates with the leading shock front and maintains the three-dimensional cellular structure of a self-sustaining detonation wave is intimately coupled to the inherent instability of the detonation wave. Erpenbeck¹⁸ and others demonstrated that the leading shock wave front is unstable to perturbations introduced into the reaction zone, because this entire region is subsonic with respect to the shock and thus such perturbations eventually overtake the shock. These perturbations occur naturally due to the turbulent nature of the interaction between exothermic chemical reactions and hydrodynamic flow¹⁹. The instability analysis of

Abouseif and Toong²⁰ demonstrated for two-dimensional detonation waves that the transverse waves of the Mach stem structure of the leading shock front develop with particular wavelengths and that a most unstable, long wavelength transverse wave is produced which governs the cell size at the shock front. What these and more recent instability analyses²¹ that used exothermic chemical reactions based on single or multiple Arrhenius reaction rates coupled to shock wave flows have neglected is the fact that the chemical energy released by these reactions is initially channeled into the vibrational modes of the various product molecules, which then undergo many collisions as they equilibrate chemically and thermodynamically as the C-J state is approached at the rear of the detonation reaction zone. If a molecule undergoes a loss of one or more quanta of vibrational energy as a pressure wavelet passes over it, the amplitude of that wavelet is increased by absorbing some of this energy⁷. Thus pressure wavelets of certain frequencies are amplified by exothermic chemical reactions as they propagate through the region of highly vibrationally excited products. Srinivasan and Vincenti²² defined conditions under which a bath of highly vibrationally excited molecules amplifies acoustic waves. Since only certain energies are released during vibrational de-excitation transitions, only wavelets with similar frequencies are amplified. These amplified wavelets then propagate to the shock front through the unreacted explosive, whose vibrational frequencies are different from those of the relaxing products and thus do not absorb energy from these wavelets. Each shock wave in the leading detonation front is continually reinforced by the arrival of these pressure wavelets.

The opposite effect, shock wave damping in a fluid that lacks vibrational energy, is a well-known phenomena²³. The pressure wave amplification process can be visualized by reversing the discussion of Zeldovich and Raiser on the damping of a wave in a gas that lacks vibrational energy²⁴. Figure 2 shows the compression-expansion cycle in pressure-volume space for a wavelet propagating in a gas that is highly vibrationally excited. The gas is rapidly compressed by the leading edge of the wavelet from point A to point B in Fig. 3 along a frozen isentrope I. The work done on the gas is equal to the area ABMN. The gas temperature and pressure increase while the vibrational energy is unchanged. Then, for the time duration of the pulse, the gas density does not change. The number of collisions is increased and the highly excited molecules can more easily undergo a transition to a lower vibrational energy level. Part of this transition energy is transferred to the translational and rotational degrees of freedom, and the temperature and pressure increase from point B to point C in Fig. 2. Since the volume does not change,

no work is done going from B to C. After the wavelet passes, the gas expands rapidly along another frozen isentrope I'. The work done by the gas is equal to area DCMN in Fig. 2. Finally there is a relatively slow transition from point D to point A at constant volume in which the pressure drops to the original value. Thus, during the expansion from C to D, the gas does more work on the surroundings than was done to it during the compression phase A to B. Therefore the gas donates to the wavelet an amount of energy ABCD in Fig. 2 equal to the difference in the work on and by the relaxing gas. The wavelet is amplified or strengthened by the vibrational de-excitation process.

As this wavelet propagates through the excited reaction products, the amplification process is repeated by the same vibrational level transition in many molecules. The time duration of the pressure pulse is critical to the amplification process. If the frequency of the wavelet is too large, its time duration is too short for a vibrational de-excitation to occur while the molecule is under compression in Fig. 2. If the frequency is too small, the time duration of the wavelet is long enough for the vibrational de-excitation energy to fully equilibrate with the translational and rotational degrees of freedom at high pressure and temperature, and no energy remains for wave amplification. Therefore the most efficiently amplified wavelet frequencies are those which match a particular vibrational state transition frequency, such as a $v=4$ to $v=3$ or a $v=4$ to $v=2$ transition in N_2 or CO, and those which match multiple transitions among a triatomic molecule's vibrational modes, such as CO_2 's four modes and H_2O 's three modes. The other wavelets whose frequencies are too low or high receive less amplification energy, rapidly decay, and die out before reaching the shock front. Wavelets whose frequencies excite the vibrational modes of the unreacted explosive are damped out before reaching the shock front.

Detonation obviously is the highest pressure, density and temperature process in which this pressure wave amplification by non-equilibrium vibrational excitation mechanism occurs. However, many other reactive flows exist in which shock, weak compression, and acoustic (sound) waves interact with exothermic chemical reactions for times long enough for amplification to occur. In the following sections, the current experimental and theoretical evidence for wave amplification in several of types of reactive flows is discussed.

SHOCK TO DETONATION TRANSITION (SDT)

The phenomenon of SDT in liquid and solid explosives is well understood because it has been studied using embedded pressure and particle velocity gauges and laser interferometry⁹⁻¹¹. For

heterogeneous solid explosives, the initial chemical decomposition is known to begin at locally heated regions called “hot spots” formed by various compression processes behind the initial shock front. These hot spots react (or fail to react) producing vibrationally excited products. The driving piston that supports the leading shock continuously sends pressure wavelets through the reacting hot spots. The wavelets are amplified by the vibrational de-excitation mechanism and overtake the leading shock front, causing it to strengthen. As the hot spots grow to consume the explosive particles between the piston and the shock front, more excited reaction product molecules are formed and more pressure wavelets are amplified. The transition to detonation occurs when a compression wave (or waves) of sufficient strength overtakes the initial shock front and causes a rapid transition to detonation. The SDT process can occur over several centimeters of shock propagation, rather than over several millimeters or less in a detonation wave⁹⁻¹¹. Figure 3 shows the SDT process in the heterogeneous solid explosive LX-17 (92.5% triaminotrinitrobenzene [TATB] and 7.5% Kel-F binder) measured using embedded particle velocity gauges and calculated using the Ignition and Growth reactive flow model⁹⁻¹¹.

In homogeneous liquid explosives or perfect crystal solid explosives, no voids are present so the shocked explosive exhibits an induction time for exothermic reaction that can be determined using high pressure, high temperature transition state theory⁶. After this induction time, rapid chemical decomposition occurs at or near the piston face. This reaction is essentially a constant volume explosion at the compression density, pressure, and temperature determined by the strength of the initial shock. This constant volume explosion creates a region of highly vibrationally excited products through which compression waves from the initiating piston must travel. These compression waves are readily amplified and rapidly form a “super detonation” wave that propagates through the compressed, unreacted explosive. The “super detonation” travels at velocities greater than C-J until it overtakes the initial shock front and then gradually slows to the C-J detonation velocity^{9,10}. No other physical mechanism for extremely rapid formation of the “super detonation” wave during homogeneous explosive SDT has ever been postulated.

There is experimental and theoretical evidence for increases in shock strength and/or shock instabilities when shock waves propagate over regions of exothermic reaction, such as flame fronts, particularly in gaseous explosives. Edwards et al.²⁵ demonstrated experimentally that shock waves could be accelerated by reacting gases in shock tubes. Soloukhin and Brochet²⁶ measured the increased instabilities and strengths of shocks that had propagated through exothermic gas mixtures. Salamandra

and Sevastyanova²⁷ followed the formation of shock waves ahead of a flame front and shock intensification during reflection back through the flame. During an experimental study of jet initiation of detonation, Thomas and Jones²⁸ observed that a shock-induced vortex formed ahead of a flame and that entrainment of hot combustion products into this vortex gave rise to localized explosions that transformed or amplified the shock into a detonation. These hot combustion products are initially formed in highly vibrationally excited states whose relaxation to lower vibrational energy levels provides the required chemical energy for the localized explosions to occur. Theoretical work on shock amplification as deflagration waves are crossed has been reported by Strachan²⁹ and Clarke et al.³⁰ Thus it appears very likely that shock wave amplification during SDT processes occurs by the same physical mechanism that is essential to detonation wave propagation.

DEFLAGRATION TO DETONATION TRANSITION (DDT)

The phenomena of DDT has often been studied in both gaseous and condensed explosives, because it is an essential process in both explosive safety (preventing it from happening) and in performance (making it happen when required). The acceleration of the deflagration wave and the formation of compression or shock waves ahead of the flame require an amplification process caused by exothermic chemical energy release, just as in detonation and SDT. In the case of DDT in gaseous and secondary condensed phase explosives, the distances involved in the reactive flow are generally greater than those for SDT and detonation. The chemical energy release during low-pressure deflagration is less concentrated than in SDT and detonation. Thus there is a lower level of vibrational excitation in the reaction products, but this excitation exists over a larger volume and a longer time since de-excitation collisions are less frequent. Thus the effects of pressure wave amplification are less pronounced in DDT processes but are observable. DDT in heterogeneous, porous solid explosives is caused by a very complex mechanism involving flame acceleration, compressive wave formation, formation of a denser plug of unreacted explosive ahead of the flame front, and shock initiation of the porous explosive upstream from this dense plug³¹. However, this complex flow does require flame acceleration and compression wave amplification by exothermic chemical reaction by highly vibrationally excited products. Some experimental and theoretical evidence for pressure wave amplification by exothermic chemical energy release during DDT processes exists. Strehlow and Cohen³² measured the continuous acceleration of a combustion flame and a reflected shock. The Schlieren images taken by Meyer, Urtiew,

and co-workers³³⁻³⁶ showed the coupled turbulent flow of deflagration and shock formation just prior to DDT. Thomas et al.³⁷ recently reviewed more recent experimental observations of the enhancement of deflagration rates when acoustic, compression or shock waves interact with exothermic chemical reactions zones. Gamezo et al.³⁸ recently reviewed theoretical work on shock-flame interactions during DDT and also stressed the close coupling of chemical energy release and pressure wave amplification. The one-dimensional simulations of Weber et al.³⁹ showed how the interaction of combustion waves and pressure waves can lead to DDT. Thus there is little doubt that passing through deflagration waves strengthens compression waves and the physical mechanism by which this occurs is most likely the same as that in SDT and detonation, i. e. the addition of one or more quanta of vibrational energy to the compression wave as a highly vibrationally excited reaction product molecule drops to a lower vibrational energy level. Subbotin⁴⁰ recently reported two initiation modes of DDT in a gaseous explosive mixture when a deflagration wave abruptly expands into a channel causing the interaction of the flame and its vibrationally excited products with expansion waves.

The most fascinating DDT processes occur in primary (very sensitive) explosives, such as lead azide and fulminate of mercury. Lead azide can undergo DDT without a measurable run distance to detonation, while most primary explosives such as fulminate of mercury and lead styphate require short distances and times for detonation wave formation⁴¹. Lead azide and some cast primary explosives undergo DDT very rapidly when ignited by a hot wire⁴². Thus the formation of a deflagration wave from a heat source, its acceleration, compression wave coalesce into a shock wave, and shock initiation of detonation must all occur very rapidly⁴². Metal azides decompose in one or a few simple reactions to form metal atoms and very highly vibrationally excited nitrogen molecules. Since nitrogen has the largest energy spacings between its vibrational levels, it can amplify pressure wavelets more efficiently and rapidly during de-excitation than other explosive products. Only the translational energy imparted to the metal atoms and the translational and rotation energies imparted to the N_2 molecules are not involved in the non-equilibrium excitation process. Therefore DDT formation in metallic azides and hydrozoic acid is limited only by the initial decomposition rates of the metal-azide bonds⁴¹. The fulminate anion is isoelectronic with the azide anion, but, since it contains C-O-N atoms, other products gases (CO, CO_2 , and H_2O if hydrogen is present) besides N_2 are formed. These products are not quite as efficient as N_2 in amplifying pressure wavelets and thus the DDT process in primaries with carbon, hydrogen and oxygen

takes slightly longer. Thus DDT in primary explosives appears to represent the fast rates of pressure wave amplification by vibrational de-excitation.

Deflagration rates of condensed phase explosives can also be measured in Diamond Anvil Cells (DAC) in which the pre-pressurized explosive sample is ignited at a small spot by a laser pulse^{43,44}. The deflagration wave velocity is then recorded on a streak camera. Deflagration rates in the pressure ranges of SDT and detonation can be obtained. Foltz⁴⁵ reported deflagration rates approaching 1 km/s at detonation-like pressures in pentaerythritol tetranitrate (PETN), which is generally considered to be at the boundary between primary and secondary explosives in sensitivity. The insensitive secondary explosives nitromethane and TATB deflagrated at tens of meters per second even at detonation-like pressures^{42,43}. Recently Esposito et al.⁴⁶ reported high pressure reaction propagation rates in octahydro-,1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) that reached a few hundred meters per second at detonation-like pressures. Explosives based on another intermediate sensitivity solid explosive, hexahydro-1,3,5-trinitro-s-triazine(RDX), appear to have deflagration rates similar to those of HMX⁴⁷. Thus the DAC laser ignited high-pressure reaction rate propagation experiments provides a “mini-DDT” test, since rapid deflagration is essential to DDT. As with detonation, SDT, and DDT, the only plausible physical mechanical mechanism for reaction rate acceleration in these milligram samples is the amplification of pressure wavelets by vibrational de-excitation of highly excited products following chemical decomposition. Species identification experiments during deflagration at high pressures in the DAC are planned.

ACOUSTIC OR SOUND WAVE AMPLIFICATION BY EXOTHERMIC CHEMICAL ENERGY RELEASE

Acoustic or sound wave amplification by exothermic chemical reactive flows have long been studied experimentally and theoretically. Experimentally, Roberts⁴⁸ demonstrated the amplification of acoustic signals by laminar pre-mixed flames and showed that the degree of amplification is inversely proportional to the frequency of the acoustic wave. As previously mentioned, the degree of “excess” vibrational energy in the reaction products of a flame will be not be as high as beyond a shock or detonation wave but will last longer since fewer de-excitation collisions will occur per unit time. Thus longer lasting (lower frequency) acoustic waves are more likely to be amplified by a flame front. Ibiricu and Krier⁴⁹ demonstrated a similar effect during solid propellant combustion. Theoretically both low and high frequency acoustic waves⁵⁰⁻⁵⁶ have been shown to be amplified by various types of exothermic reactive flows. All of these exothermic reactive flows have in common the formation of initially highly

vibrationally excited reaction product molecules, which must subsequently relax to chemical and thermodynamic equilibrium by collisions with other product molecules and expansion. The criteria for acoustic amplification set forth by Srinivasan and Vincenti²² that the vibrational temperature exceed the translational temperature and that the vibrational relaxation time is a decreasing function of temperature are met in all of these flows. Therefore the basic mechanism of wave amplification discussed for other reactive flows also applies to acoustic waves subjected to exothermic chemical energy release over a wide range of temperatures, densities, and pressures.

CONCLUSIONS

The NEZND model was formulated to identify the chemical and physical mechanisms that occur within the reaction zone of a self-sustaining detonation wave¹⁻¹¹. Exothermic chemical energy was shown to be released initially into the vibrational modes of the reaction product molecules. This large amount of vibrational energy was in “excess” of that required at the equilibrium C-J state and was sufficient to account for the chemical energy necessary to support the leading shock fronts of the detonation wave. The physical mechanism by which the “excess” vibrational energy supports the leading three-dimensional shock fronts of the detonation wave was identified as amplification of pressure wavelets of the correct frequencies by decreases in vibrational energy levels of specific modes. This pressure wave amplification was thought to be applicable to other reactive flows⁷.

Various experimental and theoretical researchers have shown that acoustic waves can be amplified by exothermic chemical energy release, that deflagration and compression waves can be accelerated by exothermic reactions, that shock waves can be amplified by flames and other exothermic reactive flows, and that DDT and SDT can occur during such amplification processes. What is lacking in these studies is consideration of the non-equilibrium processes that were identified as essential for self-sustaining detonation wave propagation based on the NEZND model. Exothermic chemical reactions in gaseous and condensed phase explosives initially populate high vibrational energy levels in their product molecules during deflagration and slow thermal decomposition just as they do in detonation. Some of this vibrational energy is available to amplify shock, compression or acoustic waves of certain frequencies passing through the excited products as they thermally and chemically equilibrate. The mechanism of wave amplification by vibrationally relaxing molecules is most efficient during DDT in primary explosives and in sustaining detonation waves at C-J velocity, but it also appears to be a general phenomenon in

many types of reactive flows involving rapid chemical energy release in the presence of acoustic, compression, and shock waves. A great deal of experimental and theoretical evidence supporting this position is discussed in this paper, but hopefully definitive experimental research will be done in this area in the near future.

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FIGURE CAPTIONS

FIGURE 1. The Non-Equilibrium Zeldovich - von Neumann-Doring (NEZND) model of detonation for condensed phase explosives

FIGURE 2. Pressure – Specific Volume states attained during a compression cycle of a vibrationally excited molecule by a pressure wavelet

FIGURE 3. Particle velocity histories for ambient temperature LX-17 shock initiated by a Kel-F flyer at 2.951 mm/ s

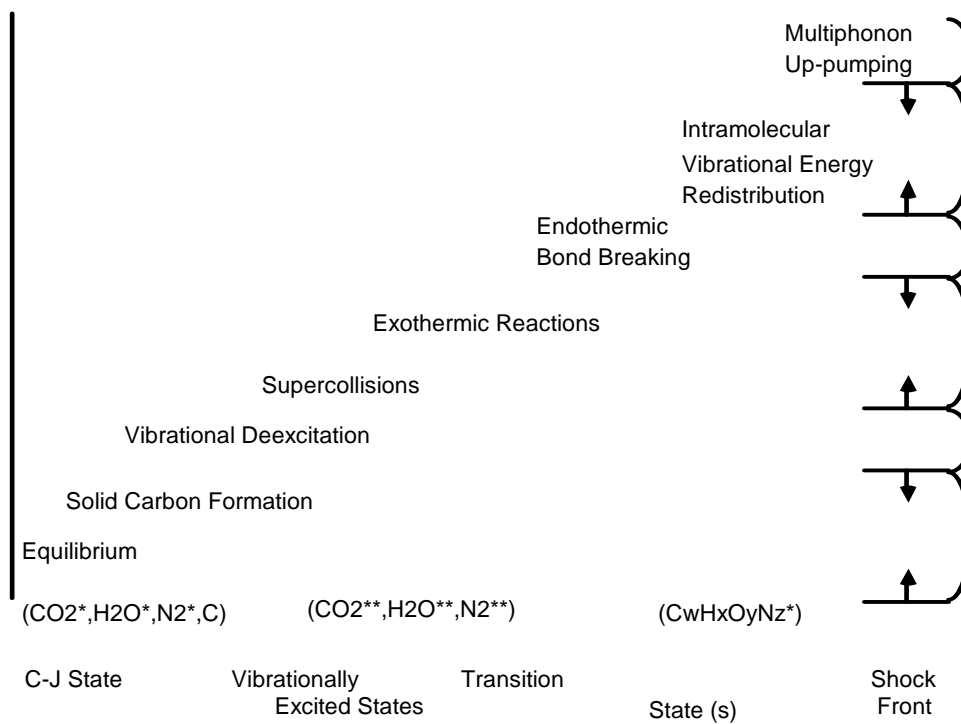


FIGURE 1. The Non-Equilibrium Zeldovich - von Neumann-Doring (NEZND) model of detonation for condensed phase explosives

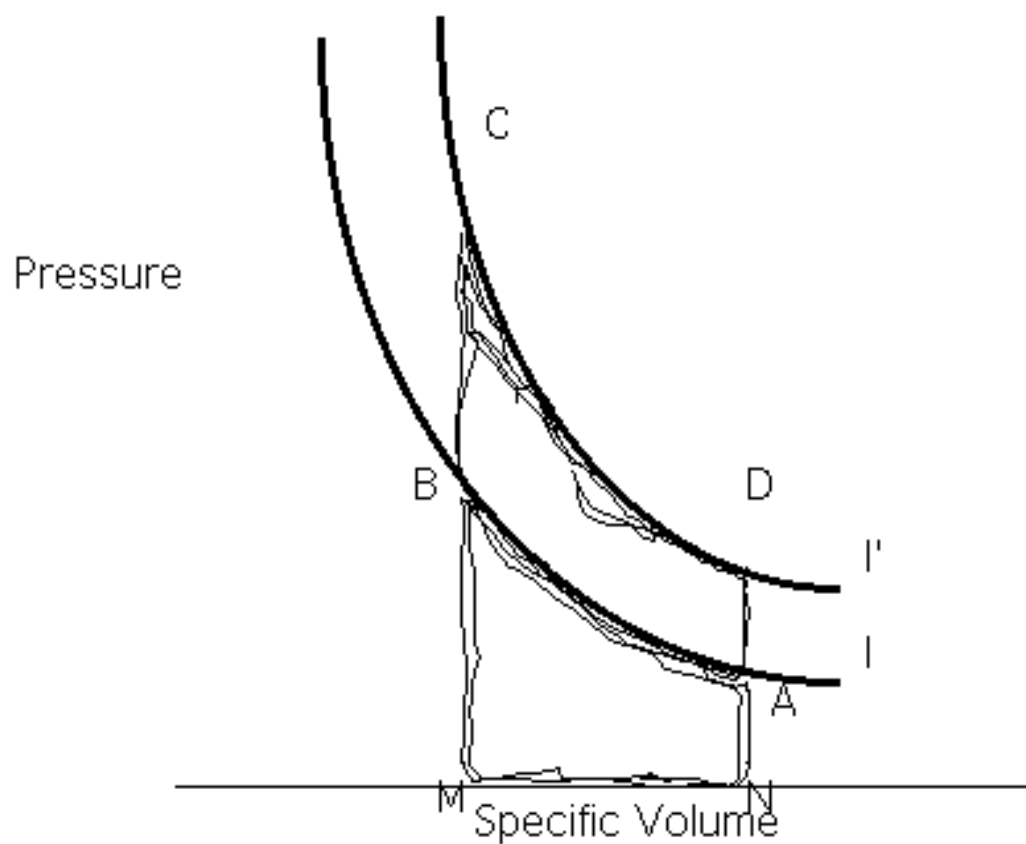


FIGURE 2. Pressure – Specific Volume states attained during a compression cycle of a vibrationally excited molecule by a pressure wavelet

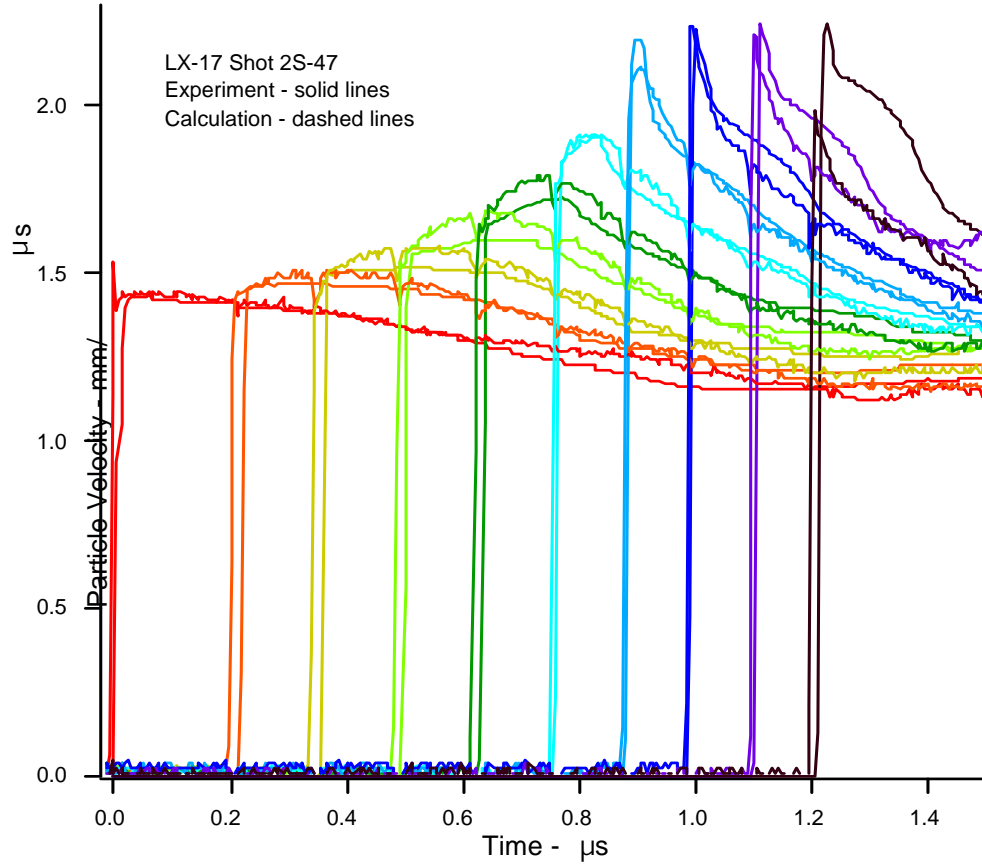


FIGURE 3. Particle velocity histories for ambient temperature LX-17 shock initiated by a Kel-F flyer at 2.951 mm/ μ s